8-Hydroxyoctanoic acid

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 99.5 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.36e-01

Confidence level: 8.02e-01

Nearest Neighbors from the Training Set

Image not found
Ethyl hexanoate
Measured: 115
Predicted: 110

Image not found
Ethyl heptanoate
Measured: 407
Predicted: 284

Image not found
2-Phenylethyl acetate
Measured: 77.6
Predicted: 98.8

Image not found
Ethyl phenylacetate
Measured: 77.6
Predicted: 103

Image not found
Aldicarb
Measured: 31.6
Predicted: 38.0